CHINESE JOURNAL OF PHYSICS VOL. 5, NC'. 2 OCTORER, 1967

Time-Dependent Variational Principle

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(Received September 25, 1967)

Variational principles for quantum theory of scattering are given. Four variational principles give the matrix elements of transition operator and two variational principles give the matrix elements of reaction operator. All the forms of the variational principles are similiar to the Schwinger variational principle for the scattering amplitude in the stationary collision theory.

I. INTRODUCTION

IN time-dependent theory of scattering, Lippmann-Schwinger theory[1] gave the variational principles for the matrix elements of scattering operator, transition operator and reaction operator. Their theory was based on the integral equations of the unitary (time-translation) operator. Altshuler and Carlson[2] derived, based on the integral equations of the wave function, a stationary expression which was similiar in form to the Schwinger variational principle for the scattering amplitude in the stationary collision theory. It is found in this paper, based on the differential equations and the integral equations for the unitary (time-translation) operators, that there are four variational principles for matrix elements of transition operator and two variational principles for matrix elements of reaction operator different from those given in Lippmann-Schwinger theory. All the forms of the variational principles given in this paper are similiar to the Schwinger variational principle.

In Sec. II, the time-dependent theory of scattering is introduced and several expressions for S-matrix are derived. In Secs. III and IV, the variational principles are formulated.

II. THEORY OF SCATTERING

The theory is formulated in the Dirac picture which is related to the Schrddinger picture by unitary transformation[3]: In the Schrödinger equation

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\Psi_S(t) &= H_S\Psi_S(t) \\ &= (H_0+H')\Psi_S(t), \end{aligned}$$

(1) B.A. Lippmann and Julian Schwinger, Phys. Rev. 79 469 1950.
(2) S. Altshuler and J. F. Carlson, Phys. Rev, 95 546 1954.
(3) S. S. Schweber: An *Introduction to Relativistic Quantum Field Theory* (Row, Peterson & Company, Elmsford, Elmsford, New York 1961) pp. 316-318.

if $$\Psi(t)=e^{iH_0t/\hbar}\Psi_S(t), \tag{1}$$

is replaced, then we get $$i\hbar\frac{\partial\Psi(t)}{\partial t}=H'(t)\Psi(t), \tag{2}$$

where $$H'(t)=e^{iH_0t/\hbar}H'e^{-iH_0t/\hbar}. \tag{3}$$

The time translation operator $U(t, t_0)$ is introduced as

$$U(t,t_0)\Psi(t_0)=\Psi(t)$$

which, from (2), satisfies the equation

$$i\hbar\frac{\partial}{\partial t}U(t,t_0)=H'(t)\,U(t,t_0).$$

It is convenient to use $t_0\longrightarrow\pm\infty$ since we usually use the time-independent state as final (or initial) state which is always refered to $t\longrightarrow\pm\infty$. Therefore[1,4]

$$U_+(t)\Psi(-\infty)=\Psi(t) \tag{4}$$

$$i\hbar\frac{\partial}{\partial t}U_+(t)=H'(t)U_+(t) \tag{5}$$

with $$U_+(-\infty)=1, \tag{6}$$

and $$U_-(t)\Psi(\infty)=\Psi(t) \tag{7}$$

$$i\hbar\frac{\partial}{\partial t}U_-(t)=H'(t)U_-(t) \tag{8}$$

with $$U_-(\infty)=1. \tag{9}$$

Integrating (5) and (8), we have

$$U_+(t)=1-\frac{i}{\hbar}\int_{-\infty}^{\infty}\eta(t-t')H'(t')U_+(t')dt' \tag{10}$$

$$U_-(t)=1+\frac{i}{\hbar}\int_{-\infty}^{\infty}dt'H'(t')U_-(t')\eta(t'-t), \tag{11}$$

where
$$\eta(t)=1 \qquad t>0$$
$$\quad\;\;=0 \qquad t<0.$$

Since the S matrix is related to $U_+(t)$ by

$$S=U_+(\infty),$$

we have, from (10)

$$S=1-\frac{i}{\hbar}\int_{-\infty}^{\infty}dt'H'(t')U_+(t'). \tag{12}$$

From (8), we have

$$-i\hbar\frac{\partial}{\partial t}U_-^{+}(t)=U_-^{+}(t)H'(t), \tag{8a}$$

(4) Der-Ruenn Su, B. S. Thesis, National Taiwan University, Taipei, Taiwan, China; 1958 (unpublished).

and after integrating, we get

$$U_{-}^{+}(t) = 1 - \frac{i}{\hbar}\int_{-\infty}^{\infty} dt' U_{-}^{+}(t') H'(t') \eta(t'-t). \tag{11a}$$

Since

$$S = U_{-}^{+}(-\infty),$$

we have from (11a)

$$S = 1 - \frac{i}{\hbar}\int_{-\infty}^{\infty} dt' U_{-}^{+}(t') H'(t). \tag{13}$$

III. MATRIX ELEMENT OF TRANSITION OPERATOR

The transition operator is difined as

$$T = S - 1.$$

From (12), we have

$$T = -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt' H'(t') U_{+}(t'), \tag{14}$$

while from (13), we have

$$T = -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt' U_{-}^{+}(t') H'(t). \tag{15}$$

The matrix element of T are, thus,

$$T_{ba} = -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt' (\varphi_b, H'(t') U_{+}(t') \varphi_a)$$

$$= -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt' (\varphi_b, H'(t') \varphi_a(t')) \tag{14a}$$

$$T_{ba} = -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt' (\varphi_b, U_{-}^{+}(t') H'(t') \varphi_a)$$

$$= -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt' (\varphi_b(t'), H'(t') \varphi_a). \tag{15a}$$

The second results of the above expressions come from (4) and (7).

In order to find another expression for T_{ba}, the equations (5) and (8a) are used:

[i] From (5), we have

$$\int_{-\infty}^{\infty} dt U_{-}^{+}(t) \left(\frac{\partial}{\partial t} + \frac{i}{\hbar} H'(t)\right) U_{+}(t) = 0. \tag{16}$$

Substituting (10) into (16), it becomes

$$0=\int_{-\infty}^{\infty}dt\,U_-^{\pm}(t)\frac{\partial U_+(t)}{\partial t}+\frac{i}{\hbar}\int_{-\infty}^{\infty}dt\,U_-^{\pm}(t)H'(t)\times$$
$$\times\left(1-\frac{i}{\hbar}\int_{-\infty}^{\infty}dt'\eta(t-t')H'(t')U_+(t')\right)$$
$$=\int_{-\infty}^{\infty}dt\,U_-^{\pm}(t)\frac{\partial U_+(t)}{\partial t}+\frac{i}{\hbar}\int_{-\infty}^{\infty}dt\,U_-^{\pm}(t)H'(t)+$$
$$+\frac{1}{\hbar^2}\int_{-\infty}^{\infty}dt\int_{-\infty}^{\infty}dt'\,U_-^{\pm}(t)H'(t)\eta(t-t')H'(t')U_+(t').$$

From (15a), we have

$$T_{ba}=-\frac{i}{\hbar}\int_{-\infty}^{\infty}dt(\varphi_b,\ U_-^{\pm}(t)H'(t)\varphi_a)$$
$$=\int_{-\infty}^{\infty}(\varphi_b(t),\ \frac{\partial\varphi_a(t)}{\partial t})+\frac{1}{\hbar^2}\int_{-\infty}^{\infty}dt\int_{-\infty}^{\infty}dt'(\varphi_b(t),H'(t)\eta(t-t')H'(t')\varphi_a(t')) \qquad (17)$$

Combining (14a)(15a) and (17), a variational principle for T_{ba} is obtained;

$$T_{ba}^{(1)}=\frac{\int_{-\infty}^{\infty}dt'(\varphi_b,\ H'(t')\varphi_a(t'))\int_{-\infty}^{\infty}dt(\varphi_b(t),\ H'(t)\varphi_a)}{-\hbar^2\int_{-\infty}^{\infty}dt(\varphi_b(t),\ \frac{\partial\varphi_a(t)}{\partial t})-\int_{-\infty}^{\infty}dt\int_{-\infty}^{\infty}dt'(\varphi_b(t),H'(t)\eta(t-t')H'(t')\varphi_a(t'))} \qquad (18)$$

The expression (18) for the correct values of $\varphi_a(t)$ acd $\varphi_b(t)$ gives the matrix element of transition operator.

[ii] From (8a), we have

$$\int_{-\infty}^{\infty}dt\left(\frac{\partial U_-^{\pm}(t)}{\partial t}-\frac{i}{\hbar}U_-^{\pm}(t)H'(t)\right)U_+(t)=0 \qquad (19)$$

Substituting (10) into (19), we have

$$0=\int_{-\infty}^{\infty}dt\frac{\partial U_-^{\pm}(t)}{\partial t}U_+(t)-\frac{i}{\hbar}\int_{-\infty}^{\infty}dt\,U_-^{\pm}(t)H'(t)\times$$
$$\times\left(1-\frac{i}{\hbar}\int_{-\infty}^{\infty}dt'\eta(t-t')H'(t')U_+(t')\right)$$
$$=\int_{-\infty}^{\infty}dt\frac{\partial U_-^{\pm}(t)}{\partial t}U_+(t)-\frac{i}{\hbar}\int_{-\infty}^{\infty}dt\,U_-^{\pm}(t)H'(t)-$$
$$-\frac{1}{\hbar^2}\int_{-\infty}^{\infty}dt\int_{-\infty}^{\infty}dt'\,U_-^{\pm}(t)H'(t)\eta(t-t')H'(t')U_+(t').$$

From (15a), T_{ba} becomes

$$T_{ba}=-\frac{i}{\hbar}\int_{-\infty}^{\infty}dt(\varphi_b,\ U_-^{\pm}(t)H'(t)\varphi_a)$$
$$=-\int_{-\infty}^{\infty}dt\left(\frac{\partial\varphi_b(t)}{\partial t},\ \varphi_a(t)\right)+\frac{1}{\hbar^2}\int_{-\infty}^{\infty}dt\int_{-\infty}^{\infty}dt'(\varphi_b(t),\ H'(t)\eta(t-t')H'(t')\varphi_a(t')). \qquad (20)$$

Combining (14a)(15a) and (20), we get another variational principle for T_{ba},

$$T_{ba}^{(2)} = \frac{\int_{-\infty}^{\infty} dt' (\varphi_b, H'(t')\varphi_a(t')) \int_{-\infty}^{\infty} dt (\varphi_b(t), H'(t)\varphi_a)}{\hbar^2 \int_{-\infty}^{\infty} dt (\frac{\partial \varphi_b(t)}{\partial t}, \varphi_a(t)) - \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' (\varphi_b(t), H'(t)\eta(t-t')H'(t')\varphi_a(t'))}. \quad (21)$$

The expression (21) for correct values of $\varphi_a(t)$ and $\varphi_b(t)$ gives again the matrix element of transition operator.

Substituting (2) into (17) and (21) in the first term in the denominator, another variational principle for T_{ba} is obtained;

$$T_{ba}^{(3)} = \frac{\int_{-\infty}^{\infty} dt' (\varphi_b, H'(t')\varphi_a(t')) \int_{-\infty}^{\infty} dt (\varphi_b(t), H'(t)\varphi_a)}{i\hbar \int_{-\infty}^{\infty} dt (\varphi_b(t), H'(t)\varphi_a(t)) - \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' (\varphi_b(t), H'(t)\eta(t-t')H'(t')\varphi_a(t'))}. \quad (22)$$

This result can also be obtained by using integral equation (10) and (11)[2,4] instead of using differential equations (5) and (8a). Combining (18) and (21) and writing in a more symmetric form, we have another variational principle,

$$T_{ba}^{(4)} = \frac{\int_{-\infty}^{\infty} dt' (\varphi_b, H'(t')\varphi_a(t')) \int_{-\infty}^{\infty} dt (\varphi_b(t), H'(t)\varphi_a)}{-\frac{\hbar^2}{2}\int_{-\infty}^{\infty} dt [(\varphi_b(t), \frac{\partial \varphi_a(t)}{\partial t}) - (\frac{\partial \varphi_b(t)}{\partial t}, \varphi_a(t))] - \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' (\varphi_b(t), H'(t)\eta(t-t')H'(t')\varphi_a(t'))}. \quad (23)$$

IV. MATRIX ELEMEMT OF REACTION OPERATOR

In order to define the reaction operator, an operator $V(t)$ is introduced(‘).

$$V(t) = \frac{2U_+(t)}{1+S} = \frac{2U_-(t)}{1+S^{-1}}, \quad (24)$$

$$V^+(-\infty) = \left(\frac{2}{1+S}\right)^+ = V(\infty),$$

$$V^+(\infty) = \left(\frac{2}{1+S^{-1}}\right)^+ = V(-\infty),$$

$$V^+(-\infty) + V^+(\infty) = V(\infty) + V(-\infty) = 2. \quad (25)$$

Then we define the reaction operator as

$$K = i[V(\infty) - V(-\infty)] = i[V^+(-\infty) - V^+(\infty)]. \quad (26)$$

From (24) and (5) or (8), we get

$$[i\hbar \frac{\partial}{\partial t} - H'(t)]V(t) = 0, \quad (27)$$

and its adjoint

$$i\hbar \frac{\partial V^+(t)}{\partial t} + V^+(t)H'(t) = 0, \quad (28)$$

Integrating (27) from $-\infty$ to t and from t to ∞, we have

$$V(t)=V(-\infty)-\frac{i}{\hbar}\int_{-\infty}^{t}dt'H'(t')V(t') \tag{29}$$

$$=V(\infty)+\frac{i}{\hbar}\int_{t}^{\infty}dt'H'(t')V(t'). \tag{30}$$

Combining these two equations, we get

$$V(t)=1-\frac{i}{2\hbar}\int_{-\infty}^{\infty}dt'\varepsilon(t-t')H'(t')V(t'), \tag{31}$$

where $\varepsilon(t)=1 \qquad t>0$

$\qquad\quad =-1 \qquad t<0.$

From (26), we get

$$K=\frac{1}{\hbar}\int_{-\infty}^{\infty}dtH'(t)V(t). \tag{32}$$

Integrating (28) from $-\infty$ to t and from t to ∞, we have

$$V^{+}(t)=V^{+}(-\infty)+\frac{i}{\hbar}\int_{-\infty}^{t}dt'V^{+}(t')H'(t') \tag{33}$$

$$=V^{+}(\infty)-\frac{i}{\hbar}\int_{t}^{\infty}dt'V^{+}(t')H'(t'). \tag{34}$$

From (26), (33) and (34), we have

$$K=\frac{1}{\hbar}\int_{-\infty}^{\infty}dt'V^{+}(t')H'(t'). \tag{35}$$

From (32) and (35), K_{ba} is expressed in

$$K_{ba}=\frac{1}{\hbar}\int_{-\infty}^{\infty}dt'(\varphi_b,\ H'(t')V(t')\varphi_a)$$

$$=\frac{1}{\hbar}\int_{-\infty}^{\infty}dt'(V(t')\varphi_b,\ H'(t')\varphi_a). \tag{36}$$

In order to find another expression for K_{ba}, equation (27) is used;

$$\int_{-\infty}^{\infty}dtV^{+}(t)(\frac{\partial}{\partial t}+\frac{i}{\hbar}H'(t))V(t)=0.$$

By (31), we substitute in the integral equation,

$$0=\int_{-\infty}^{\infty}dtV^{+}(t)\frac{\partial V(t)}{\partial t}+\frac{i}{\hbar}\int_{-\infty}^{\infty}dtV^{+}(t)H'(t)(1-\frac{i}{2\hbar}\int_{-\infty}^{\infty}dt'\varepsilon(t-t')H'(t')V(t'))$$

$$=\int_{-\infty}^{\infty}dtV^{+}(t)\frac{\partial V(t)}{\partial t}+\frac{i}{\hbar}\int_{-\infty}^{\infty}dtV^{+}(t)H'(t)+$$

$$+\frac{1}{2\hbar}\int_{-\infty}^{\infty}dt\int_{-\infty}^{\infty}dt'V^{+}(t)H'(t)\varepsilon(t-t')H'(t')V(t').$$

From (36), we have

$$K_{ba}=\frac{1}{\hbar}\int_{-\infty}^{\infty}dt\,(V(t)\varphi_b,\ H'(t)\varphi_a)$$
$$=i\int_{-\infty}^{\infty}dt\,(V(t)\varphi_b,\ \frac{\partial V(t)}{\partial t}\varphi_a)+$$
$$+\frac{i}{2\hbar}\int_{-\infty}^{\infty}dt\int_{-\infty}^{\infty}dt'\,(V(t)\varphi_b,\ H'(t)\varepsilon(t-t')H'(t')V(t')\varphi_a). \quad (37)$$

Combining (36) and (37), it yields a variational principle for the matrix element K_{ba};

$$K_{ba}^{(1)}=\frac{\int_{-\infty}^{\infty}dt\,(\varphi_b,\ H'(t)V(t)\varphi_a)\int_{-\infty}^{\infty}dt'\,(V(t')\varphi_b,\ H'(t')\varphi_a)}{i\hbar^2\int_{-\infty}^{\infty}dt\,(V(t)\varphi_b,\ \frac{\partial V(t)}{\partial t}\varphi_a)+\frac{i}{2}\int_{-\infty}^{\infty}dt\int_{-\infty}^{\infty}dt'\,(V(t)\varphi_b,\ H'(t)\,\varepsilon(t-t')H'(t')V(t')\varphi_a)} \quad (35)$$

Since the only trial function existed here is $V(t)$, the expression $K_{ba}^{(1)}$ for the correct value of $V(t)$ is the metrix element of the reaction operator K_{ba}.

Substituting (27) into (38), we have

$$K_{ba}^{(2)}=\frac{\int_{-\infty}^{\infty}dt\,(\varphi_b,\ H'(t)V(t)\varphi_a)\int_{-\infty}^{\infty}dt'\,(V(t')\varphi_b,\ H'(t')\varphi_a)}{\hbar\int_{-\infty}^{\infty}dt\,(V(t)\varphi_b,\ H'(t)V(t)\varphi_a)+\frac{i}{2}\int_{-\infty}^{\infty}dt\int_{-\infty}^{\infty}dt'\,(V(t)\varphi_b,\ H'(t)\varepsilon(t-t')H'(t')V(t')\varphi_a)} \quad (39)$$

Again, the expression $K_{ba}^{(2)}$ for the correct value of $V(t)$ is K_{ba}. The equation (39) can also be derived from the integral equations for $V^{+}(t)$ and $V(t)$.